Definition of Strategies for Production and Consumption of Sustainable Aviation Fuels in Portugal

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Abstract

Development of strategies for the production and consumption of sustainable aviation fuels (SAF) in Portugal, based on an extensive interdisciplinary literature review, referring to existing strategies and the state of the art. Three potential conversion routes were selected: Hydrotreated Esters and Fatty Acids (HEFA), Alcohol-to-Jet (ATJ) and Fischer-Tropsch (FT). For an initial approximation to the environmental impacts of SAF, an analytic production model was elaborated to determine the best use of resources to reduce greenhouse gases (GHG) emissions. The model applied to these routes and their resources allowed for an optimization via linear programming with two objective functions, GHG reduction and cost. Two scenarios resulted that maximize the reduction of GHG emissions (12 to 18%) and minimize cost. A techno-economic model was developed, dedicated to ascertaining the mass and energy balances of the three associated biorefineries (ATJ-E, ATJ-B and FT), as well as their efficiency and conditions for economic viability. From the latter model it emerged that the ATJ-E biorefinery is currently the most competitive. A sensitivity analysis shows that with hydrogen at 5.2 €/kg, no modeled biorefinery is viable, while at 3.2 €/kg all would be viable. With hydrogen at 6.5 €/kg, the minimum SAF selling price ranges from 0.60 to 0.81 €/L. Finally, a strategy was suggested based on a unique strategic matrix and composed of 3 phases: study, demonstration and implementation of biorefineries, based on scenarios obtained from the first model and deepened in the techno-economic model.

Keywords: energy, SAF, aviation, biofuels, strategy, sustainability

1 INTRODUCTION

Nowadays, the aviation industry is one of the pillars of our civilization. The jet propulsion of aircraft used by the aviation industry operates through the combustion of products derived from fossil fuels. As such, the industry's operations result in greenhouse gas (GHG) emissions, mainly carbon dioxide, $\mathrm{CO_2}$, that contribute to climate change. The International Panel on Climate Change (IPCC) estimates that GHG emissions from the aviation industry are 2% of the total emissions produced by the human species. If the industry were a country, it would be the 8th largest emitter of $\mathrm{CO_2}$, and given its size and long-term growth forecasts, emissions could reach 2700 Megatons by 2050 (IRENA, 2017) if no further action is taken.

Pre-emptively, industry organizations, airlines and aircraft manufacturers have set goals in order to mitigate the climate consequences of aviation. Some common goals among various entities are increased energy efficiency and carbon-neutral growth starting in 2020. Despite advances in technologies such as electric and hydrogen-powered aircraft, the energy density of these technologies severely limits their near-term implementation in aviation. Due to the high lifespan of 25 years, on average (Bureau of Transportation Statistics, 2018), of a commercial aircraft, added to the fact that huge quantities are already sold and there are orders with decade-long margins (CAPA - Centre for Aviation, 2018), the industry's need for high energy density liquid fuels is likely to remain for the coming decades. Thus, it is imperative to use so-called drop-in fuels, deployable directly throughout the infrastructure and interchangeable with current fossil fuel-derived products.

Sustainable Aviation Fuels (SAF) are defined as certified, drop-in fuels that meet sustainability standards. These fuels bring significant advantages to the industry, including the opportunity to simultaneously reduce GHG emissions and diversify fuel supply, maintain current infrastructure, support the development of local circular economies and sustainable development. However, due to obstacles such as high cost of production, competition with biodiesel, and the absence of policies to encourage implementation, their adoption has been slow. In this context, the objective of this study is the definition of strategies for the consumption and production of SAF in Portugal. It is essential to study the strategies already adopted around the globe through a literature review, as well as the state of the art of the production of these fuels, to understand how production in Portugal can be executed. Identifying value chains and analysing them from an environmental impacts and economic viability point of view is also fundamental.

2 LITERATURE REVIEW

2.1 ANALYSIS OF EXISTING STRATEGIES

In 2016, the International Civil Aviation Organization (ICAO) signatory states, including Portugal, adopted CORSIA (Carbon Offsetting and Reduction Scheme for International Aviation), a regime of market-based measures for international aviation (ICAO, 2019). Under the CORSIA scheme, offsetting of CO_2 emissions is to be done on the basis of the operator's annual emissions and an airline may purchase emission units to neutralize its own emissions. The development and use of SAF is included in the set of measures defined by ICAO to achieve sustainability in the sector. To this end, CEF (CORSIA Eligible Fuels) were defined as eligible fuels for the CORSIA scheme, thus offering operators the opportunity to reduce their emission offset requirements.

The International Renewable Energy Agency (IRENA) published a technology report on biofuels in aviation in 2017 (IRENA, 2017). Important findings of the study include the identification of obstacles such as the high cost of production of biofuels, which is doubly penalizing due to the fuel being one of the main expenses of airlines. Other obstacles also include competition with biodiesel, difficulty in creating national policies, which is further coupled with the lack of policy incentives for production, and finally, jet fuel not being taxed on international flights (European Commission, 2019b).

Regarding the European continent, in addition to the ETS (European Emissions Trading Scheme), an emissions trading system that includes airlines and operates in the European Economic Area (EEA), meeting 45% of the Union's GHG emissions (European Comission, 2020), there is the Renewable Energy Directive (RED II). The RED II defines as a goal a 32% share of renewable sources in the overall energy of the European Union for 2030, with each member state being responsible for the National Energy and Climate Plan (APREN, 2018). Regarding the transport sector, the target is set at 14% of fuels from renewable sources, and similarly to other strategies, it does not require renewable fractions in air transport. However, the directive does value their production: "*The contribution of renewable non-food fuels supplied to these sectors (aviation and maritime) will count for 1.2 times their energy content.*" (European Commission, 2019a). Other relevant measures in the directive include the requirement that alternative fuels reduce GHG emissions by 65% and the limitation of fuels with high indirect land-use change (ILUC) risks.

The FlightPath initiative, through the ESFERA (European Sustainable Fuel Routes for Aviation) project, has recently developed a document that identifies and analyses the main existing national strategies in the European continent (ESFERA, 2020). The study shows examples such as the UK, where the government has provided 22 million pounds of funding for projects to develop low carbon waste-based fuels for air transport and heavy vehicles. Other countries, such as France and Netherlands, announced that taxes would be introduced on civil aviation. Norway will impose on airlines operating in its airspace the mandatory use of biofuels starting with the amount of 0.5% in 2019, also setting a goal that 30% of aviation fuels sold by 2030 be biofuels. Similar to the UK, the Swedish government will fund the research and development of projects studying SAF, there will also be a group consisting of representatives from the entire SAF production chain, whose goal will be to evaluate and propose steps for sustainable aviation. In 2019, a report was produced at the request of the Swedish government, which also proposes to make the use of SAF mandatory, the aim is to reach 100% in 2045 (FlightPath, 2019). Similarly, to the innovation group practiced in Sweden, Spain has started dialogues with the main national operators, concluding mandating 2% SAF by 2025.

International aviation is the domain of ICAO and consequently of the CORSIA regime. Domestic flights in Portugal are covered by the ETS. If the SAF produced complies with the RED II sustainability criteria, then credits are also created that can be traded under the ETS (ESFERA, 2019). Furthermore, the Portuguese National Energy and Climate Plan for 2030 (PNEC2030) proposes to achieve by 2030 a 45% to 55% reduction in GHG emissions compared to 2005, mentioning incentives for investment in advanced transportation biofuels, which valorise national resources and waste, promoting a circular economy. The plan foresees that in 2025, 255 ktoe of 1st generation biofuels and 94 ktoe of advanced biofuels will be consumed, metrics that reach 136 and 155 ktoe, respectively, in 2030 (República Portuguesa, 2019).

In 2017, a National Plan for the Promotion of Biorefineries was prepared (Pinto *et al.*, 2017). In legislative terms, energy valorisation biorefineries, i.e., optimized to produce bioenergy products, will require stable policy incentives of medium and long duration. In addition, as mentioned before, the main expenses in the production of advanced biofuels are related to the cost of biomass, investment (CAPEX) and operation (OPEX) of biorefineries. In this sense, opportunities to decrease expenses include co-production of value-added chemicals and use of low-cost waste biomass. Some other advantages include evolution in territorial cohesion, creation of skilled and unskilled jobs, development of alternative markets and use of the practical knowledge of the paper industry already established.

After studying existing strategies, several obstacles to the introduction of SAF are observed. The high cost of production, mainly associated with the acquisition of raw material, also dependent on the initial capital required. Also associated with this obstacle is competition with biodiesel, in that production is relatively cheaper and supported by policy frameworks that are not yet common for SAF. Directly related is the difficulty experienced by individual countries in creating national policies capable of encouraging the production of biofuels specifically for aviation, translating into a lack of incentives for production. The absence of SAF mandates, in international strategies such as CORSIA, ETS, and RED II, is also a barrier, adding to the problem the fact that jet fuel is not taxed on international flights.

Regarding existing opportunities, the most obvious ones are the reduction of GHG emissions and other air pollutants (Pereira Gaspar, 2016). Another advantage is the existence and certification of the technology, to which is also added the precedent of biofuels penetration in road transport. Regarding the frameworks in political strategies, the introduction of SAF benefits by being an alternative to the ETS and CORSIA. SAF also benefit from the difficulty of technological transformation in air transport in the short term (unlike road transport), so that some European countries are already giving preference to requiring these alternative fuels in domestic air transport. In economic terms, there is a chance that GHG emissions from fossil sources will progressively become more expensive, so SAF may become a more viable option in the future. Alternatively, there could be an introduction of specific subsidies for SAF, making their production more attractive.

2.2 ANALYSIS OF THE STATE OF THE ART OF SAF PRODUCTION

In 2009, the first production chain of an alternative aviation fuel was approved by the American Society for Testing and Materials (ASTM International). Today, there are 6 processes certified by the institution, representing 4 families of conversion pathways (ICAO, 2019):

- Paraffinic kerosene synthesized via the Fischer-Tropsch method (FT-SPK) and high aromatic SPK via the same method (FT-SPK/A);

- Paraffinic kerosene synthesized from esters and hydroprocessed fatty acids (HEFA-SPK);

- Iso-paraffinic fuels synthesized from hydroprocessed fermented sugars (SIP-HFS);

- Aviation fuel synthesized from alcohol, specifically ethanol and isobutanol (ATJ-SPK);

In 2009, ASTM approved the certification of FT-SPK. According to ASTM standard D7566, fuels produced from this process can be blended in an amount up to 50% (by volume) with traditional fuels (Hitchcock, 2019). The process involves gasification of biomass at high temperatures to obtain syngas. Due to the presence of contaminants, e.g. alkali metals, purification follows and the syngas is converted, via a catalytic reaction (FT synthesis), into a mixture of liquids and gases with hydrocarbon chains of different sizes and, depending on the reaction parameters and refining, SAF can be produced (ICAO, 2018). SPK based fuels alone do not have the minimum amount of aromatic content, so interest has arisen in developing synthetic paraffinic kerosene with high aromatic content (SPK/A), also via FT, so that it is possible to increase the percentage of SAF used (Torres, 2014). In 2015, this production chain was approved by ASTM International, Annex 5 of the ASTM D7566 standard, and although it is limited to a 50% blend it may eventually reach 100% (ICAO, 2018).

Hydroprocessed esters and fatty acids can also be converted to SPK in a process approved in 2011 by ASTM standard D7566, Annex 2 (Hitchcock, 2019). The standard allows a volumetric amount of 50% in the fuel mixture and the feedstocks encompass bio-oils, animal fats and other recyclable oils such as used cooking oil (UCO) (ICAO, 2018). The process requires hydrogenation, forming hydrocarbons that are subsequently refined to achieve the properties that comply with the standard (Pereira Gaspar, 2016). This production chain accounts for the largest share of aviation biofuels currently produced, however the same chain produces biodiesel, so production of the latter is ultimately favoured due to the low cost of production and the already established market (IRENA, 2017).

Annex 3 of the ASTM D7566 standard, incorporated in 2014 concerns SIP-HFS and indicates that their use is only allowed up to volume fractions of 10% (Hitchcock, 2019). The cause of this limitation is the unsuitability of the product (farnesane), different from typical hydrocarbons, with respect to the specifications of the standard (Pereira Gaspar, 2016). As the name implies, this route involves the biological fermentation of sugars, through microorganisms, producing farnesene, which is then reacted with hydrogen to generate farnesane (IRENA, 2017). Feedstocks used contain sugars, examples are lignocellulosic biomass such as forest and agricultural residues (ESFERA, 2019).

The fifth addition (appendix 5) to the ASTM D7566 standard was the production of SPK from alcohol, specifically the butanol isomer, isobutanol. This route was approved in 2016 and was initially allowed a 30% volume fraction in the mixture (Hitchcock, 2019). However, in 2018 the use of another alcohol, ethanol, was approved and the permitted volume fraction was increased to 50% (Lanzatech, 2018). After appropriate pre-treatment for the biomass used, fermentation of the respective alcohol occurs in a tank via microorganisms, in the case of isobutanol, strains of *Escherichia coli* and *Saccharomyces cervisae* fine-tuned to better tolerate butanol as it is produced (Roussos et al., 2019). The next step requires dehydration, forming an olefinic gas that goes through oligomerization leading to compounds with higher molecular weights, followed by hydrogenation (Pereira Gaspar, 2016).

In the context of ascertaining which SAF conversion pathways are promising in Portugal, technological and economic feasibility, but also GHG emissions, are the chosen criteria. Regarding technology, applying a Fuel Readiness Level (FRL) approach (CAAFI, 2019) is useful to clarify the condition of the production chains, as shown on table 1. In relation to GHG, RED II defines a minimum reduction of 65%, defining the minimum limit. Table 2 displays GHG emission reference quantities for the conversion pathways under commercial implementation, as well as the respective percentage reductions when compared to the ICAO-defined fuel standard value of 89 g CO_{2_e}/MJ.

From table 1 it is possible to infer that the SIP route suffers from stagnation in its technological development, which also explains the difficulty in finding information about this production route in the literature. A possible cause for the lack of significant advances is the 10% limit on blending with fossil fuel and the competition, in terms of raw materials (fermentable sugars and hydrogen), with the ATJ conversion route which allows reaching a blend of 50%, thus being a more interesting investment. Hence, the SIP pathway is disregarded in this work. Through table 2 it becomes unequivocal that the FT and HEFA conversion routes can be implemented according to the requirements of RED II. Nevertheless, possible technological improvements in the ATJ pathway could allow for greater emission reductions which would make this conversion pathway attractive, considering how close it is to reaching the 65% minimum.

In terms of technology readiness, HEFA, is well established, while the other two pathways, one biochemical conversion, ATJ, and the other thermochemical, FT, are expected to reach FRL level 9, represented as an operational commercial plant, in 2021. These three conversion pathways are made up of technologies already established in several other industries, so the ultimate test of both pathways will be to combine these technologies, on a large scale, in an efficient and economically viable manner, from biomass, thus overcoming the difficulties inherent to these feedstocks, such as moisture content, ash content and heterogeneity. It is also important to note that the ATJ and FT routes already led, in 2019, the installed capacities in planning stages, combined being worth a total of 550,000 tons of annual production (Sustainable Aviation, 2020).

Table 1 - FRL of SAF production routes certified by ASTM.

Production Routes	2015 (Mawhood *et al.*, 2016)	2016 (Alves *et al.*, 2016)	2021
FT-SPK	7-8	7-8	8
HEFA-SPK	6-9	8	9
SIP-HFS	5-7	7-8	7
ATJ-SPK	4-6	6	8

Table 2 - Standard GHG emissions of selected SAF production routes (Sustainable Aviation 2020).

Production Routes	GHG emissions ($\mathrm{g\ CO_{2_e}/MJ}$)	GHG reduction (%)	Feedstock
FT-SPK	13.7	84.6	Woody residues
HEFA-SPK	14.0	84.3	UCO and animal fats
ATJ-SPK	35.0	60.7	Corn Stover

All three routes use different types of biomass as feedstock, the common hypothesis of hydrogenation and fractional distillation as final steps and the possibility of syngas fermentation. Thus, the three routes complement each other, and there are even some examples of studies on hypothetical integrated biorefineries (Klein *et al.*, 2018). Table 3 contains the mass yields of each of these routes from feedstocks similar to those previously mentioned in table 2.

Table 3 - Yields of conversion (adapted) (Alves et al., 2016).

Production Route	Mass Yield (g SAF/ g feedstock)	Feedstock
HEFA	0.494	Oils
ATJ	0.207	Fermentable Sugars
FT	0.151	Lignocellulosic Biomass

3 METHODOLOGY

3.1 ANALYTIC PRODUCTION MODEL

An analytical production model was created in order to evaluate the potential for SAF production in Portugal, the GHG emissions associated with this production and its energy allocation to each pathway, exclusively from feedstocks in table 3.

SAF, as drop-in fuel, was assumed to have identical properties to traditional jet fuel (set out in table 4). Excluding the monthly production maximum (peak of 200 million litters), whose respective emissions are approximately 615 thousand tons of $\mathrm{CO_{2_e}}$, calculated with the emission standard mentioned above, all values used were mentioned earlier in this paper. The HEFA route used UCO, while the ATJ and FT routes used corn stover and lignocellulosic forestry waste from eucalyptus, respectively.

The model parameters are set out as follows: maximum monthly production of 200 million litters per month, resulting in 615 thousand tons of $\mathrm{CO_{2_e}}$ for traditional jet, using a lower heating value (LHV) of 42.8 MJ/kg and a density of 807.5 $\mathrm{kg/m^3}$. From table 3, yields are extracted, with 0.121 being used for ATJ starting from corn stover due to an estimate of 65% fermentable sugars within, extracted with a 90% yield. From table 2, GHG emissions patterns are extracted.

Table 4 - Important properties in traditional jet (adapted) (Vásquez, Silva and Castillo, 2017).

Property	Limit	Jet-A1
Aromatic volume (%)	Maximum	26.5%
Flash point (ºC)	Minimum	38
Density at 15ºC ($\mathrm{kg/m^3}$)	Min.	775-840
Freeze point (ºC)	Max.	-47
LHV ($\mathrm{MJ/kg}$)	Min.	42.8

In brief, the inputs to the model are the desired monthly SAF production, either in MJ, ktoe or million litters and the allocation of this production (as a function of energy), as a percentage, to each of the three pathways. The model uses the parameters discussed above and returns primarily, for each conversion pathway and the totals (both SAF produced and traditional jet fuel) the energy (MJ/month), mass (kton/month), volume (million litters/month), emissions (kton $\mathrm{CO_{2_e}}$ /month), amount of feedstock required (kton/month), and finally, the GHG reduction compared to the traditional monthly peak production, in percent.

The first approach was to quantify the maximum installed capacity and emissions. Given that SAF production is limited to 100 million litters per month (50% volume of traditional jet (Joint Organisations Data Initiative, 2021)), this is necessarily the theoretical maximum. Thus, **Scenario 1** uses the input of a production that reaches 100 million litters per month, completely (100%, in the model input) assigned to the FT conversion pathway, since it minimizes GHG emissions. The outputs of scenario 1 are in table 5.

It is clear from the results that the maximum reduction of GHG emissions that Portugal can achieve in the aviation industry will be 42.33%. This would require more than 500 thousand tons of lignocellulosic waste, including eucalyptus, every month. It should be added that during the course of this work, biorefineries using the FT conversion route have not yet been demonstrated for a scale of 100 million litters per month.

In **Scenario 2**, 155 ktoe per year is chosen as the energetic production of SAF, defined in the PNEC as desired for advanced biofuels in 2030. Regarding the allocation of this production, 100% is allocated to the HEFA pathway, since it is already industrially established (FRL of 9) and its product is eligible both for RED II and as a CEF, thus of guaranteed technological maturity. Scenario 2 is also shown on table 5.

In order to characterize, through this initial approximation methodology, the true national potential for SAF production, the model was used in reverse. That is, the monthly feedstock mass values obtained from the National Plan for the Promotion of Biorefineries were introduced as inputs and the monthly production and the percentages dedicated to each of the conversion routes were returned as outputs. The chosen feedstocks were corn stover (118.08 kton/month), eucalyptus residues (37.33 kton/month) (Pinto *et al.*, 2017) and UCO (13.08 kton/month) (APA, 2019).

Table 5 – Analytical Production Model outputs for Scenarios 1 and 2.

Outputs	Scenario 1		Scenario 2	
	FT	Total	HEFA	Total
Energy (TJ/month)	3456.10	6912.2	540.80	6912.20
Mass (kton/month)	80.75	161.50	12.64	161.50
Volume (ML/month)	100	200	15.65	200
GHG emissions (ktonCO_{2_e}/month)	47.35	354.94	7.57	574.63
Feedstock mass (kton/month)	534.77		25.58	
GHG reduction (%)		42.33		6.59

The results of this **Scenario 3** are presented in table 6. The national potential for SAF production thus stands at 32.69 million litters per month, taking into account the feedstocks studied. This number is equivalent to 16.35% of the monthly peak volume of 200 million litters, so it is a significant amount that would represent a reduction in GHG emissions of 11.70%. The percentages of this production, in energy, allocated to each conversion pathway would be 24.48% for the HEFA pathway, 54.17% for the ATJ pathway and 21.35% for the FT pathway, equating to 8, 17.71 and 6.98 million litters per month, respectively. The main weakness of this scenario is that the feedstock for the HEFA conversion technology is already destined for biodiesel production (APA, 2019).

With the information gathered and the production simulation model built, it is possible to optimize resources through linear programming. The solution to this linear programming problem is simplified because the monthly quantities of raw materials are the variables and, with only two, the solution can be obtained graphically. In the context of this work, reducing GHG emissions is the main objective in order to make the industry more sustainable. Conversely, the minimization of feedstock costs is desirable for the economic viability of biorefineries

The cost of lignocellulosic waste from eucalyptus is 51.03 EUR/ton (Alves et al., 2016) and, although there is no market for corn surplus, the cost associated with this raw material is 40.68 EUR/ton (Edwards, Hart and Leibold, 2012). The cost function, in the group of equations 1, is obtained immediately given the costs of each raw material, were I_{ATJ} and I_{FT} are the monthly biomass inputs of each pathway (kton/month).

However, GHG emissions reduction (1) is a bit more complex. This function was derived from computing the monthly standard jet emissions, by subtracting the produced mass of both SAF pathways and adding their respective emissions as a function of input biomass mass. Thus, X_{Total} (kton CO_{2_e}/month) represents monthly emissions as a function of SAF production.

In order to define restrictions, the maximum biomass quantities available where chosen: R_1 limits I_{ATJ} up to 118.08 kton/month and R_2 limits I_{FT} up to 37.33 kton/month. R_3 is an inferior limit, requiring at least 12.64 kton/month of SAF production while R_4 and R_5 restrict the problem only to positive inputs quantities R_3 is defined based on scenario 2 outputs, being the minimal advanced biofuels production accepted. Figure 1 illustrates this multi-objective linear programming graphically, the pink area represents the feasible solutions, and the vertices are the points where the objective functions find their optimal solutions. The application of these coordinates to the objective functions is done in table 7.

Table 6 - Analytical Production Model outputs: Scenario 3.

Outputs	HEFA	ATJ	FT	Total
Energy (TJ/month)	276.57	612.01	241.21	6912.20
Mass (kton/month)	6.46	14.30	5.64	161.50
Volume (ML/month)	8.00	17.71	6.98	200
GHG emissions (ktonCO_{2_e}/month)	3.87	21.42	3.30	543.23
Feedstock mass (kton/month)	13.08	118.08	37.32	
GHG reduction (%)				11.70

$$C\ (kEUR/month) = 40.68 \cdot I_{ATJ} + 51.30 \cdot I_{FT} \qquad (1)$$

$$X_{Total} = 615.19 - 0.28 \cdot I_{ATJ} - 0.49 \cdot I_{FT}$$

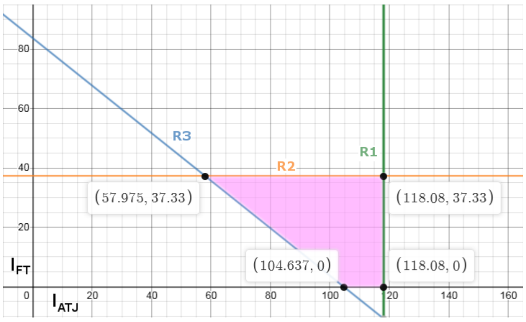

Figure 1 - Graphical solution of the linear programming problem.

From table 7 it results that, as expected, the point that minimizes the function X_{Total} is point B, thus achieving the greatest reduction of GHG emissions in relation to the monthly peak. In turn, the point that minimizes function C is point D, which would imply monthly raw material costs around 4 million euros. With the two solutions for each function being far apart, it becomes even more important to pay attention to the other points. Point A, with the cost very similar to the minimization of the cost function of point D, achieves a more attractive percentage reduction in GHG emissions, although still far from the maximization of reductions of point B. This similarity of costs between A (57.98;37.33) and D (104.64;0) is interesting because if the cost difference is considered negligible, point A in the context of this study, given the superior GHG reduction, would be the optimal solution of the cost function. Since A and B are on the same line, if one day production reaches the production values of point B, it will have to have passed through point A. Thus, points A and B were used to create **Scenarios 4** and **5**, respectively. For this, the analytical production model was used again in an inverse manner, as was done to develop scenario 3.

Table 7 - Solutions to the linear programming problem.

Point	A	B	C	D
I_{ATJ} (kton/month)	57.98	118.08	118.08	104.64
I_{FT} (kton/month)	37.33	37.33	0.00	0.00
C (MEUR/month)	4.26	6.71	4.80	4.26
X_{Total} (ktonCO_{2_e}/month)	580.67	563.84	582.13	585.89
GHG reduction (%)	5.61	8.35	5.37	4.76

For scenario 4, which minimizes the cost function and acquiesces to the energy minimums defined by PNEC2030, based on point A, the model attributes 55.5% of the energy produced to the ATJ route and 44.5% to the FT route. Monthly production reaches 15.67 million litters. For scenario 5, which maximizes the cost function and minimizes the GHG emissions function, based on point B, the model attributes 71.7% of the energy produced to the ATJ route and 28.3% to the FT route. Monthly production reaches 24.69 million litters. In scenarios 4 and 5, SAF accounts for 7.80% and 12.35% of the peak jet fuel production. The respective GHG emission reductions are 5.59% and 8.33%.

When the average monthly demand for jet fuel in Portugal is considered (Joint Organisations Data Initiative, 2021), scenario 4 is also characterized by a minimum monthly reduction of GHG emissions of 7% and can still reach a maximum of 12%. The average monthly GHG reduction is around 9.09%. As to scenario 5, the minimum monthly GHG emissions reduction is around 10% and reaches a maximum of 18%, with an average GHG emission reduction value of 13.54%. This scenario maximizes the GHG reduction, the use of available resources and their cost.

3.2 TECHNO-ECONOMIC MODEL

In order to study scenarios 4 and 5 from a mass and energy as well as financial point of view, a more complete model, described in this section, was developed. In the design of this model, the basic idea is to use as a single input the results of the analytical production model, specifically the exact amount of raw material to be consumed each month, so as to satisfy scenarios 4 and 5. The techno-economic model returns, as outputs, the mass and energy balances of the production pathways, the requirements in terms of other important resources such as hydrogen and water, surplus electricity (if this is the case) and data on the economic viability of the biorefineries considered.

To understand the energy and mass balances, step by step, of each production route, the techno-economic modelling requires a heuristic methodology, given the absence of information. Thus, new estimates were sought for the mass yields of these two pathways, based on the average mass yields found in the literature, for each step of the production pathway for which information is available, in order to reach the production function. Through the results of the mass balances, the energy balances and consequently the requirements, surplus electricity, efficiencies, emissions and economic viability are calculated.

Table 8 shows the average mass yields of each production step within the ATJ production family. These average yields were computed from several literature sources [(Neuling and Kaltschmitt, 2015), (Straathof, 2014), (Alves *et al.*, 2016), (Jong *et al.*, 2015), (Geleynse *et al.*, 2018), (Klein *et al.*, 2018), (Han, Tao and Wang, 2017), (Doliente *et al.*, 2020) and (Roussos *et al.*, 2019)]. Further, hydrolysis and fermentation were grouped as pre-treatment, so were dehydration, oligomerization and hydrogenation grouped as ATJ upgrading and finally the distillation was divided into 3: SAF, Diesel and Gasoline, with densities of 837 and 770 $\mathrm{kg/m^3}$ for the latter two (Wang *et al.*, 2016). With the mass yields and densities defined, by using the LHVs of table 9, the energy balances are computed from the mass balances.

Table 8 - Average mass yields of the ATJ route steps for ethanol (ATJ-E) and isobutanol (ATJ-B).

Production Step	Average Mass Yields	
	ATJ-E	ATJ-B
Hydrolysis	0.5900	
Fermentation	0.4413	0.3495
Dehydration	0.8317	0.9465
Oligomerization	0.9847	0.9334
Hydrogenation	0.9950	
Distillation	0.9900	
SAF	0.6433	0.7000
Diesel	0.1533	0.0000
Gasoline	0.2033	0.3000
$(\mathrm{g_{SAF}}/\mathrm{g}_{fermentable\ sugar})$	0.2226	0.2775

The existing literature does not allow to build databases on the FT route, especially considering the gasification of eucalyptus residues. Furthermore, while the ATJ pathway is of linear design, the FT pathway offers variations that involve fundamental decisions such as the oxidizing agent, type of gasifier, desired syngas composition, and catalysts for the FT reaction. Thus, it is important to establish main steps of this route and order them: pre-treatment (mechanical), gasification, syngas cleaning, FT reaction and distillation (hydrogenation followed by distillation for SAF, diesel and gasoline).

Table 9 - LHVs of products and raw materials used.

Product/Resource	LHV (TJ/kton)	Source
Corn Stover	17.45	(Huang *et al.*, 2009)
Eucalyptus Residues	18.82	(Nwokolo, Mukumba and Obileke, 2020)
Fermentable Sugars (Glucose)	14.24	(Phyllis, 2021)
Ethanol	27.00	(Wang *et al.*, 2016)
Isobutanol	36.00	
Diesel	43.00	
Gasoline	47.00	
$\mathrm{H_2}$	120.00	(Gray *et al.*, 2021)

Once the main steps have been established, the next step is to determine the mass yields of each. Similar to what was done for the ATJ route, the mechanical pre-treatment has an assumed yield of 95%. Gasification is next and from equations in 2 and 3 it emerges that the cold gas efficiency (CGE) and carbon conversion efficiency (CCE) must agree. By calculating $\dot{m}_{syngas}$ in kton/month, the mass yield of this step is arrived at. Given that CGE and CCE are dependent on each other, setting a value within the ranges of 50 to 80% for CGE will result in a value for CCE, and, with that value also being within the ranges of 90 to 99% for CCE, there will be agreement (Arena, 2012). However, there are 3 unknown variables in these equations: $\dot{m}_{syngas}$, PCI_{syngas} and $\dot{m}_{carbon(syngas)}$.

$$CGE = \frac{\dot{m}_{syngas} \cdot PCI_{syngas}}{\dot{m}_{biomass} \cdot PCI_{biomass}} \tag{2}$$

$$CCE = \frac{\dot{m}_{carbon(syngas)}}{\dot{m}_{carbon(biomass)}} \tag{3}$$

To determine the 3 unknown terms, it is unavoidable to turn to the literature. However, due to the lack of options, the first decision influencing the design of this biorefinery is made, table 10 contains the mass and mole fractions of the syngas composition from the gasification of eucalyptus residues in a fixed-bed reactor with downdraft flow and using atmospheric air as oxidizing agent. By using the mass fraction values in Table 10 the syngas LHV can be determined (Nwokolo, Mukumba and Obileke, 2020). With the LHVs of 50.016 and 10.112 for methane and carbon monoxide (Turns, 2012), respectively, as well as the tabulated value above for the PCI of hydrogen, it is possible to calculate the PCI of the obtained syngas. Thus, PCI_{syngas} is equal to 5.90 TJ/kton.

With PCI_{syngas} found, the calculation of the carbon flux, by mass, in the syngas follows. This value is computed by using $\dot{m}_{syngas}$ and again the mass fractions in the syngas composition stated in table 10. With $\dot{m}_{carbon(syngas)}$ defined as a function of $\dot{m}_{syngas}$, which in turn is defined as a function of CGE, and CCE defined as a function of $\dot{m}_{carbon(syngas)}$, assigning a value to CGE allows both efficiencies and both mass flows of syngas and carbon in syngas to be characterized. As such, it was chosen to use the model to assign the minimum possible value to the CGE efficiency that minimizes the CCE, but keeps both results consistent, so as not to overestimate future model results. Thus, a CGE of 0.74 returns a CCE of 0.90, minimizing the acceptable range for the CCE. Between the gasification and the FT reaction, syngas cleaning takes place, for which a yield of 90% was assumed.

Table 10 - Composition of syngas from gasification of eucalyptus residues (adapted) (Nwokolo, Mukumba and Obileke, 2020).

Fraction	Mass (%)	Molar (%)
H_2	1.90	22.88
CO	28.90	24.71
CH_4	1.40	2.06
CO_2	18.20	9.84
N_2	49.50	40.50

Regarding the FT reaction, assuming that the carbon dioxide contained in the syngas is recycled back to the gasifier, assuming a 0.4 yield (Klein *et al.*, 2018) for the single-pass conversion of carbon monoxide, the FT mass yield is defined as a function of $\dot{m}_{carbon(syngas)}$ (Gruber *et al.*, 2019). These liquids undergo a hydrogenation process that requires 0.10 gram of hydrogen per gram of FT wax (Alves et al., 2016). Finally, hydrogenation is assumed to have a similar mass yield to the ATJ route of 99.5% and, similarly, a 99% yield for distillation. In the absence of percentage distributions of the distillation products, the model uses the distribution of the ATJ route for ethanol, available in table 8, and which already encompasses the distillation yield. Regarding ATJ requirements, 0.528 TJ of H_2 per TJ of SAF, 6.1 litters of water per litter of SAF and 226 kWh per ton of corn stover of electricity surplus were assumed (Han, Tao and Wang, 2017). Finally, biorefinery efficiencies are established (equations 4 and 5), based on mass and energy balances, were x can be any product or their total sum.

$$\eta_{M_x} = \frac{M_x}{M_i} \tag{4}$$

$$\eta_{E_x} = \frac{E_x + E_{ele}}{E_i + E_{H_2}} \tag{5}$$

In order to make a realistic estimate of the costs associated with biorefineries, the power law, with p being 0.84, is applied (Tsagkari *et al.*, 2016). The power law (6) is useful as it allows one to derive the costs of the biorefineries in question from the costs (c) of similar biorefineries described in the literature, provided that the scale, s, for example in terms of feedstock consumed monthly, is also available. Term t is a correction.

$$\frac{c_1}{c_2} = \left(\frac{s_1}{s_2}\right)^p \cdot t \tag{6}$$

Tables 11 and 12 contain the parameters inserted in the extrapolation of the ATJ and FT routes with the power law, s_1 is determined via simple conversion, according to scenarios 4 and 5. By applying the power law to each of the routes, the CAPEX and OPEX are obtained. Since the model specifies the quantity of products, if values for sales prices are defined, annual revenues can easily be calculated. Likewise, since the model also specifies the quantity of resources used monthly, if values for purchase prices are defined for, i.e. hydrogen and raw materials, the annual costs are obtained by adding up to the respective OPEX values. Once the annual revenues and expenses are defined, it is possible to develop the model to characterize economically the three biorefineries. Assuming that the revenues and expenses are constant over the lifetime of the biorefineries, and that the initial investment is made in year 0, the NPV is straightforward. The IRR assumes the same circumstances as the NPV. To complete the model, values of 10% and 30 years were set as interest rate for the project and its lifetime in years. Equating the NPV to zero and solving for the price of SAF per litter, we arrive at the Minimum SAF Selling Price (MSAFSP). This is a useful metric because it indicates the minimum price at which SAF should be sold for the biorefinery in question to be economically viable.

Table 11 – Parameters applied ATJ (Geleynse *et al.*, 2018).

Parameters	ATJ-E	ATJ-B	Units
s_2	435.00		Sugar ton/day
CAPEX	77.40	74.60	M$
OPEX	15.80	16.50	M$/year
t	0.89		

Table 12 - Parameters applied in the FT power law (Jong *et al.*, 2015).

Parameters	FT	Units
s_2	85.70	kton/month
CAPEX	327.00	M$
OPEX	65.40	M$/year
t	0.94	

4 DISCUSSION AND STRATEGIES

Given the proprietary nature of the new technologies developed in SAF production, finding large datasets is impractical. Thus, a heuristic methodology was used to develop the techno-economic model. The techno-economic model, which assumes constant circumstances in the operating conditions of the 3 conceptualized biorefineries, after their construction, so that their production functions can be linearly simplified, needs only the inputs taken from the **analytical production model**: 57.99 kton/month of corn stover for the ATJ route and 37.29 kton/month of eucalyptus residues for the FT route, in **scenario 4** and, 118.05 kton/month of corn stover for the ATJ route and 37.37 kton/month of eucalyptus residues for the FT route, in **scenario 5**. The model returns mass and energy balances, mass and energy efficiencies, hydrogen and water consumption, electricity export (if applicable), GHG emissions and the economic viability, under identical circumstances to allow comparisons, of the 3 biorefineries in question (ATJ-E, ATJ-B and FT), in the 2 scenarios obtained from the use of the analytical production model.

The relative errors of the techno-economic model compared to the analytical production model are satisfactory, with the maximum being 6% for the ATJ-E biorefinery and the minimum being 1.39% for the FT biorefinery mass yield.

In scenario 4, The ATJ-E biorefinery dominates the ATJ-B one in all efficiencies except those referring to gasoline, another example of the superior selectivity of isobutanol. Moreover, it is interesting to note that in terms of SAF energy and mass efficiencies, the two biorefineries are very close, an evidence in favour of the balance between the two due to the advantageous fermentation of ethanol and the superior selectivity of isobutanol. Assuming an $\mathrm{H_2}$ price of 4 EUR/kg, ATJ-E is superior to ATJ-B in annual expenses and costs. However, given that the two are of the same scale, and that the ATJ-E biorefinery has a better annual balance despite consuming more hydrogen, it can be said to be the more efficient route in economic, mass and energy terms. This is due not so much to the subtly higher mass yield of the ATJ-E route, but rather to the fact that the price of jet fuel is much cheaper than gasoline or diesel, so the biorefinery that produces less SAF (in terms relative to distillation) will have an economic advantage. Hence, it is not surprising that the ATJ-E biorefinery is dominant in all economic feasibility parameters. Special attention should be paid to the MSAFSP of 0.265 EUR/L which implies that the ATJ-E biorefinery is already very competitive today. Similarly, the MSAFSP of 0.429 EUR/L also indicates that the ATJ-B biorefinery could achieve a positive NPV soon, being very close to the current price.

In scenario 5, the economies of scale of biorefineries are shown as a great advantage in financial terms, making the positive balance between annual revenues and expenses even greater, especially in the case of the ATJ-E biorefinery. $\mathrm{H_2}$ seems to be by far the main annual expense, representing a share of 54.88 and 52.80% in biorefineries ATJ-E and ATJ-B, respectively, if a 4 EUR/kg price is assumed. Scenario 5 also shows the importance of economies of scale, attributing an NPV of approximately 382 million euros to the ATJ-E biorefinery and an IRR of 25.6%. The MSAFSPs also became more competitive, with the ATJ-B biorefinery also benefiting from the economies of scale and achieving a positive NPV with an IRR of about 11.8%.

The FT biorefinery is more efficient with respect to energy-focused chemical products, the exception to the rule being efficiency with respect to diesel, outperformed by the ATJ-E biorefinery. On the financial side, the FT biorefinery has the shortest annual profit margin and will therefore have the worst performance. This is despite requiring less $\mathrm{H_2}$ in absolute terms (111 TJ/month) and in relative terms, as it accounts for 45.30% of the annual expenses. The small scale, relative to the ATJ pathway biorefineries in scenarios 4 and 5, also makes this difficult. In addition, the high CAPEX and more expensive feedstock also penalize margins, despite good efficiencies. With a negative NPV of approximately 74 million and the worst IRR of all biorefineries in both scenarios, the economic viability of the FT route is the least competitive. However, the MSAFSP of 0.49 EUR/L is promising for the future.

Given the importance of the price of $\mathrm{H_2}$ for biorefineries, a sensitivity analysis indicates that under scenario 4 and the same circumstances, a price of 4.9 EUR/kg of $\mathrm{H_2}$ would make the ATJ-E biorefinery economically unviable, requiring an MSAFSP higher than 0.40 EUR/L. Similarly, under the same circumstances and in scenario 5, a price of 5.2 EUR/kg of $\mathrm{H_2}$ makes the most competitive ATJ-E biorefinery unviable, keeping the MSAFSP equivalent to 0.40 EUR/L. Contrarily, should the cost of $\mathrm{H_2}$ drop and reach 3.2 EUR/kg, the FT biorefinery would become viable in both scenarios.

Thus, this analysis finishes knowing that only below 4.9 EUR/kg of $\mathrm{H_2}$ would the modeled biorefineries become economically viable if the prices of the energy products they produce are maintained. Below 3.2 EUR/kg of $\mathrm{H_2}$, all the modeled biorefineries are viable at today's SAF, gasoline and diesel prices. It is also known that in the transition from scenario 4, to scenario 5, which concerns exclusively the installed capacity of the ATJ route, the initial biorefinery should be expanded from the (57.99 to 118.05 kton/month of corn stover), to benefit enormously from economies of scale. It is also known that in economic terms the ATJ-E biorefinery should be chosen over the ATJ-B biorefinery if current circumstances persist.

Finally, with $\mathrm{H_2}$ at 4 EUR/kg and in scenario 4, only the ATJ-E biorefinery is economically viable. Under these conditions an MSAFSP of about 0.43 EUR/L would be required to make the ATJ-B biorefinery viable and a value of 0.49 EUR/L to make the FT route viable. Also, with $\mathrm{H_2}$ at 4 EUR/kg, but now in scenario 5, thanks to economies of scale the ATJ-B biorefinery is already viable, generating a considerable NPV. However, the ATJ-E biorefinery is the most competitive, with an NPV of around 382 million euros.

Thus, to optimize resources, scenarios 4 and 5 should be targets to be achieved in any strategy. Given the unpredictable nature of large-scale biorefinery development, the defined strategy should contain redundancies to prevent complete failure. Therefore, a strategy of 3 distinct phases is suggested: In the 1st phase a working group is created, with all stakeholders of the future SAF production chains, attempting the development of preliminary studies regarding technology, business models, environmental impacts and political strategies, with the objective of financing, building and disseminating the necessary knowledge for the implementation, in the most efficient way, of the next phases of the strategy. In the 2nd phase two demonstration plants are built for the ATJ and FT routes so that they can be tested in an integrated way. The 3rd phase is the implementation of the biorefineries depending on the results of the second phase, according to the strategic matrix presented in figure 2. In this matrix, values from 1 to 4 refer to demonstrations, progressively more complex, achieved by the respective experimental plants. For the ATJ pathway, 1 is the demonstration of ethanol production from residual biomass such as corn stover, 2 is the demonstration of ATJ-SPK production, 3 is the production of ATJ-SPK from syngas, and 4 is the demonstration of ATJ-SPK production via isobutanol. Analogously, for the FT route, 1 is demonstration of syngas production from lignocellulosic residues, 2 the demonstration of the entire production chain from the same residues, 3 is the gasification of lignin from corn stover, and 4 is the demonstration of the entire production chain from MSW.

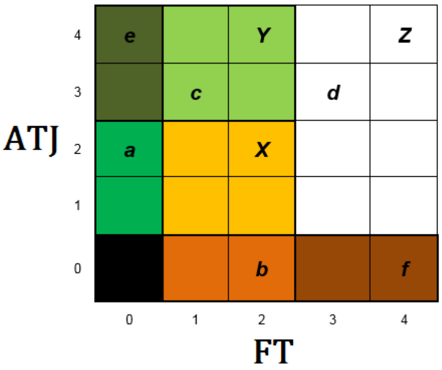

Figure 2 - Strategic Matrix of SAF implementation.

The letters in the strategic matrix are "win" conditions that allow implementing advances in the production of SAF in Portugal. With a demonstration of 2 in the ATJ pathway, "***a***" indicates the possibility of building the 1st ATJ biorefinery, in this case ATJ-E. In turn, "***b***" indicates the possibility of building the 1st FT biorefinery, while "***X***" represents that both conditions to execute scenario 4 are met, thus reaching the minimum acceptable production of SAF in Portugal. As for "***c***" and "***d***", they represent integrations in the biorefineries of the different routes, namely syngas fermentation and lignin gasification, respectively. Finally, "***e***" indicates the possibility to empirically compare the performances of the ATJ-E and ATJ-B pathways, and "***Y***" represents the possibility to move with certainty to scenario 5, thus optimizing the use of corn stover and eucalyptus residues. However, if demonstration 4 of the FT pathway is achieved, "***f***", the national potential for SAF production is expanded, resulting in a possible scenario 6 ("***Z***"), where there is the possibility of using MSW as feedstock in the FT pathway.

This phased strategy promotes cooperation between actors and minimizes risks because only success in each phase will allow for the next one. The working group created in the 1st phase will have to be successful and highly productive for the 2nd phase to be initiated, and, in turn, it will be the success of the 2nd phase that will define the future of the 3rd phase and consequently of the production of SAF in the country.

5 CONCLUSIONS

In order to define strategies for the production and consumption of SAF in the Portuguese Republic, a comprehensive and interdisciplinary approach was developed. First, an extensive literature review was conducted, divided in two parts. The first one, referring to the already existing strategies at international, European and domestic level. The second part of the literature review was dedicated to the study of the state of the art of SAF production. Furthermore, from the state of the art analysis of the four families of SAF production, it was possible to determine, based on environmental performance and technology readiness level, the three most promising families to be launched in the short-medium term (HEFA, **ATJ** and **FT**), something essential in the context of climate change.

The potential value chains of the three promising families was identified and modelled in the Portuguese context. Based on the characterization of the national installed capacity and with some data extracted directly from the literature, an **analytical production model** was developed, for an initial approximation to the environmental impacts of SAF. The objective was to determine the best allocation to each promising pathway and the monthly production of SAF adequate to the resources available in the country. Given competition with biodiesel, SAF production via HEFA was immediately compromised, despite being the most industrially established conversion family. In contrast, the ATJ and FT pathways, which dominate in future planned capacities, fit the available resources in the country, corn stover and eucalyptus residues, respectively. The analytical production model applied to these routes and their respective resources allowed for the evaluation of the national potential for SAF production, the production energy allocations and the environmental impacts. In addition, it also allowed an optimization via the application of a linear programming problem with multiple (two) objective functions. From this innovation emerged two scenarios that minimize each of the chosen objective functions (GHG emissions and cost) and ultimately represent a range between the minimum acceptable by policy makers for the production of advanced biofuels, in which SAF is included, to the maximum consumption for the feedstocks in question.

The characteristics of the two scenarios were essential to develop the techno-economic model. **Scenario 4** states a monthly production of 15.67 million litres with 44.5 and 55.5% allocated in energy terms to the FT and ATJ routes, respectively. The same scenario introduces monthly GHG reductions between 7 and 12%, with an average of 9.09%. **Scenario 5**, on the other hand, would produce 24.69 million litres of SAF per month (with allocations of 28.3 and 71.7%, respectively) and monthly GHG reductions between 10 and 18% with the average value of 13.54%.

Knowing the scale of the scenarios to be studied, as well as the feedstocks, a heuristic methodology was chosen to create the **techno-economic model**, given the scarcity of useful information. The objective of the detailed model was to ascertain the mass and energy balances of the three associated biorefineries (ATJ-E, ATJ-B and FT), as well as their efficiency and constraints on economic viability. The economic aspect was addressed once again with heuristic methodology, namely the power law. The relative errors between the analytical production model and the techno-economic model were minimal, demonstrating that the heuristic methodology allowed the development of a model as useful in terms of results as those in the literature. It emerged from the techno-economic model that the ATJ-E biorefinery is the most competitive. The main discrepancy with the literature was the financial burden of clean hydrogen, as a value of €4 per kg was assumed. From this came a brief sensitivity analysis that offers further introspections: with hydrogen at €5.2 per kg, no modelled biorefinery is viable, while at €3.2 per kg, all would be viable. With hydrogen at €6.5 per kg, MSAFSPs range from €0.60 to €0.81 per litter.

Finally, a strategy was suggested based on a unique strategic matrix and composed of 3 phases: study, experiment and implementation of biorefineries. This implementation is based on the scenarios obtained from the analytical production model and further developed in the techno-economic model, underlining the originality of this study, by developing production scenarios via optimization of resources, costs and environmental impacts, deepened by a techno-economic model for each biorefinery contained in the scenarios in question and then used to suggest strategies for production and consumption of SAF.

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